

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123591.D
 Acq On : 16 Apr 2021 14:20
 Operator : JU/CG
 Sample : M2048-15
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-14.5-15.0

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	17	rVB	2846898	3851715	48.39%	6.519%
2	4.457	398	403	409	rBV	97035	112534	1.41%	0.190%
3	5.087	501	510	518	rVB	432011	598487	7.52%	1.013%
4	5.487	573	578	581	rBV	7474478	7212749	90.61%	12.207%
5	6.498	744	750	753	rBV	7013217	7448150	93.57%	12.605%
6	6.869	809	813	816	rBV	1501230	1277501	16.05%	2.162%
7	6.928	820	823	832	rBV	227873	208156	2.61%	0.352%
8	7.434	903	909	911	rBV	4711495	4884159	61.36%	8.266%
9	7.510	917	922	929	rBV2	78560	97128	1.22%	0.164%
10	8.151	1025	1031	1034	rBV	2190709	1709188	21.47%	2.893%
11	9.233	1210	1215	1218	rBV	8784554	7514015	94.39%	12.717%
12	9.504	1258	1261	1265	rBV	659919	488569	6.14%	0.827%
13	9.622	1278	1281	1284	rBV	227892	173672	2.18%	0.294%
14	9.910	1326	1330	1334	rBV	2210396	1825261	22.93%	3.089%
15	10.704	1460	1465	1468	rBV	6534578	5659906	71.10%	9.579%
16	11.398	1579	1583	1587	rBV	2222475	2008348	25.23%	3.399%
17	11.933	1667	1674	1691	rBV	896737	915014	11.49%	1.549%
18	12.539	1774	1777	1781	rBV	131026	122958	1.54%	0.208%
19	12.721	1803	1808	1818	rBV2	92740	112269	1.41%	0.190%
20	12.998	1850	1855	1858	rBV	8671052	7960355	100.00%	13.472%
21	13.227	1889	1894	1909	rBV	104042	125535	1.58%	0.212%
22	13.568	1950	1952	1955	rBV	122407	98682	1.24%	0.167%
23	13.904	2005	2009	2025	rBV2	568661	1092066	13.72%	1.848%
24	14.051	2029	2034	2037	rBV	1649247	1562189	19.62%	2.644%
25	14.221	2059	2063	2065	rBV	167256	150234	1.89%	0.254%
26	14.527	2111	2115	2118	rBV	174686	165731	2.08%	0.280%
27	14.839	2163	2168	2174	rBV	132296	163967	2.06%	0.277%
28	15.186	2223	2227	2232	rVB	113492	127774	1.61%	0.216%
29	15.533	2281	2286	2291	rBV	921790	1216335	15.28%	2.059%
30	15.580	2291	2294	2299	rVB3	74665	102076	1.28%	0.173%
31	16.298	2412	2416	2420	rVB5	69531	102911	1.29%	0.174%

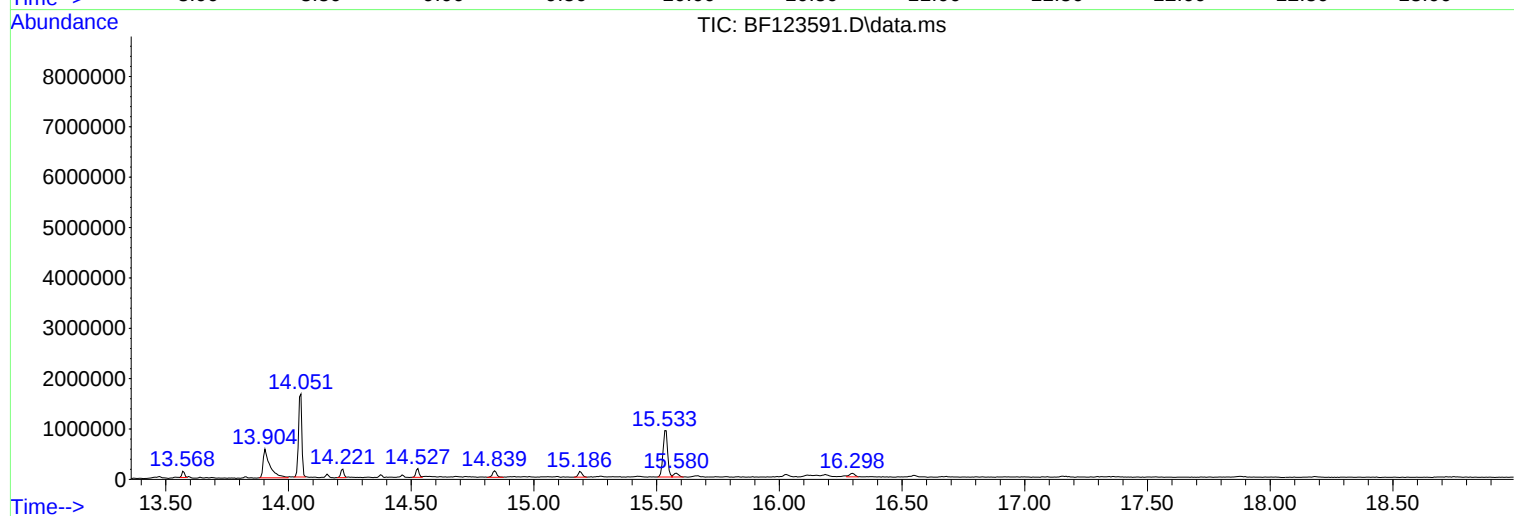
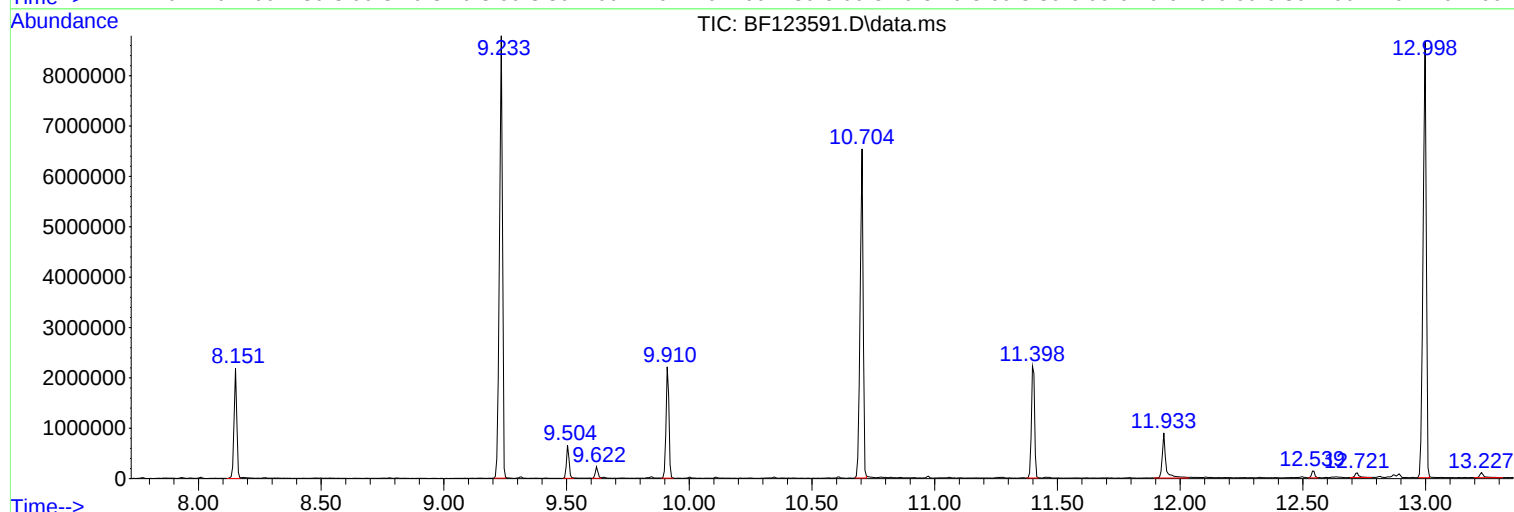
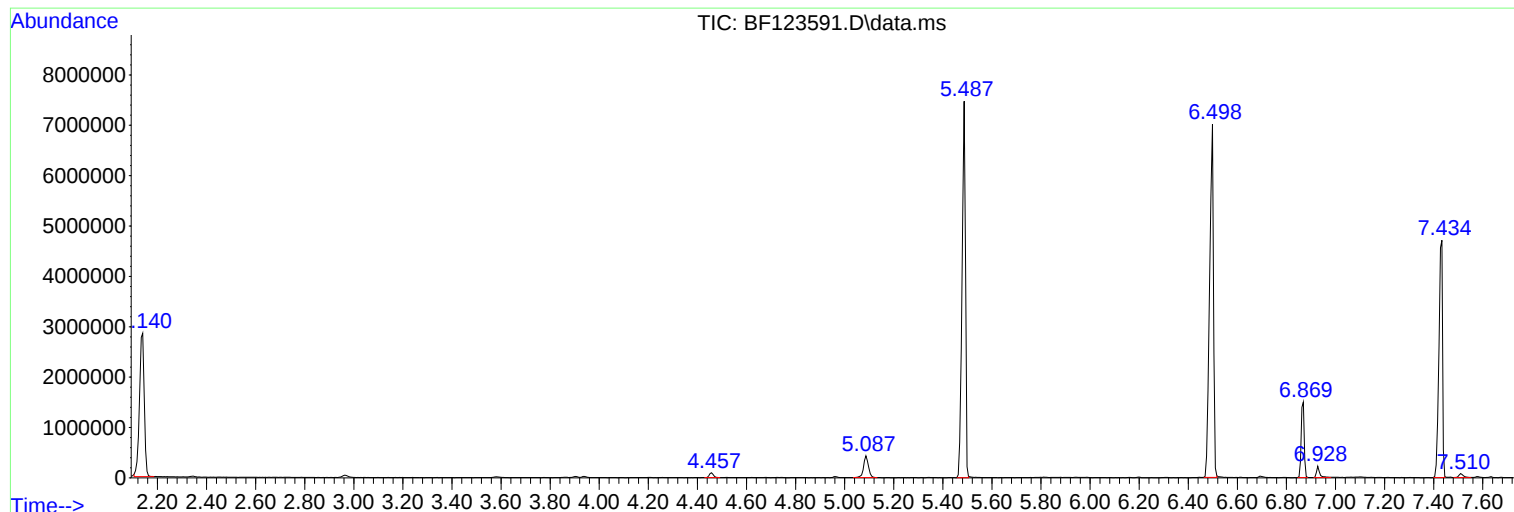
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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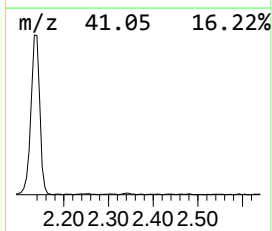
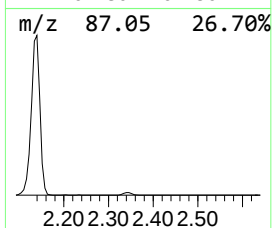
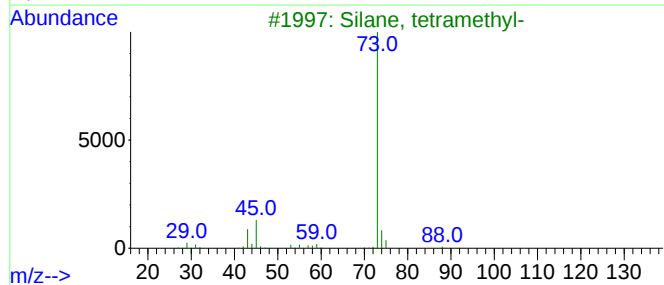
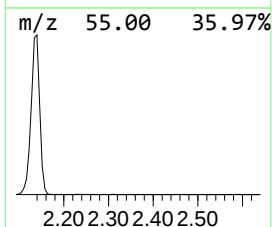
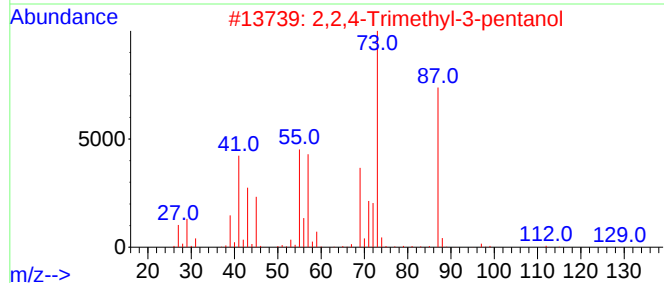
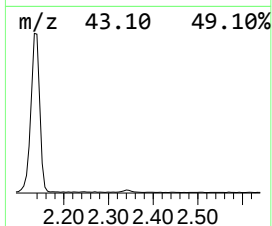
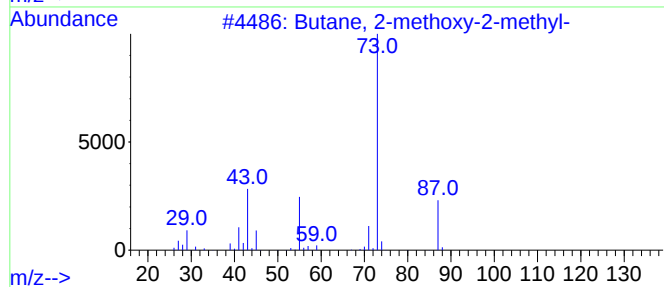
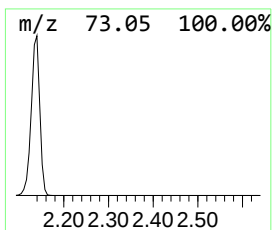
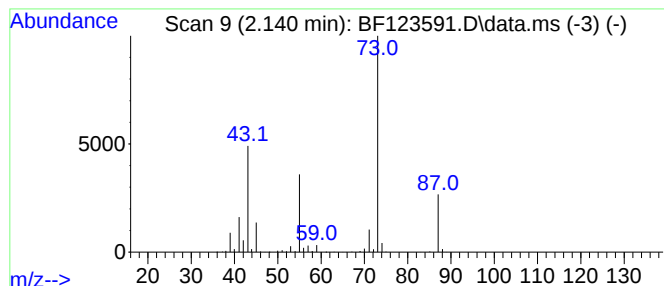
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	60.30 ng	3851720	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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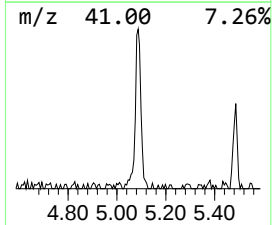
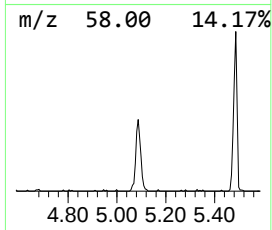
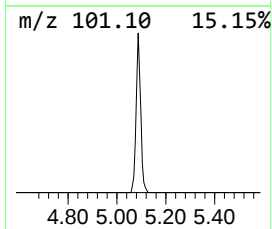
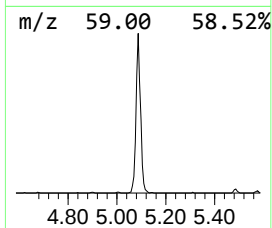
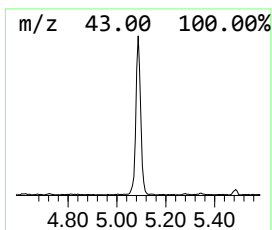
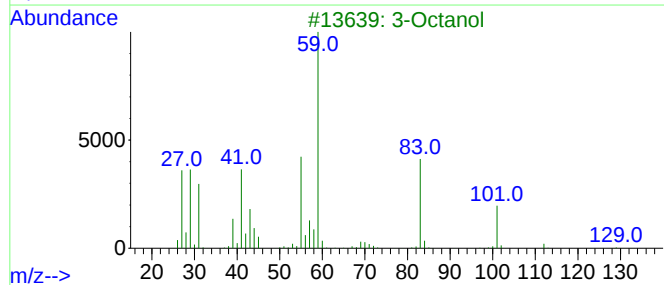
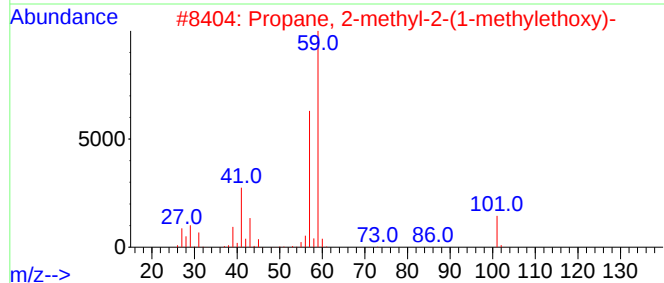
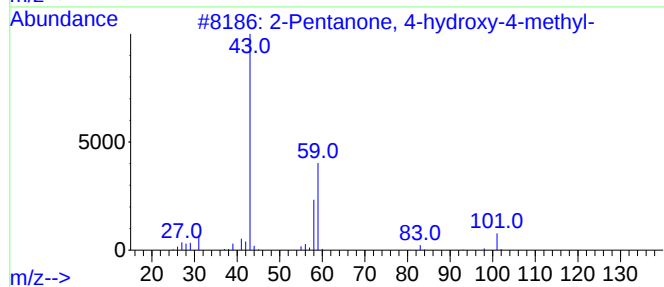
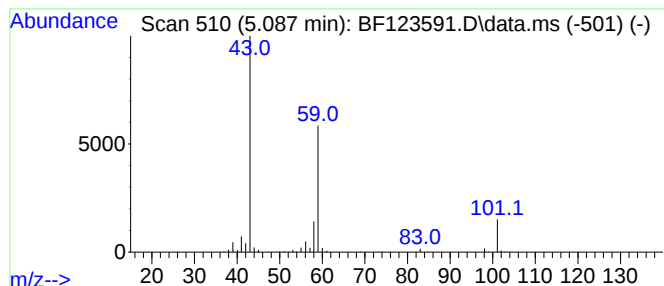
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	9.37 ng	598487	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Octanol	130	C8H18O	000589-98-0	33		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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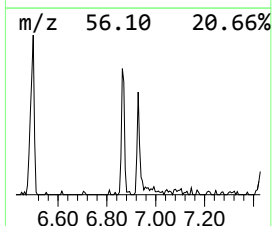
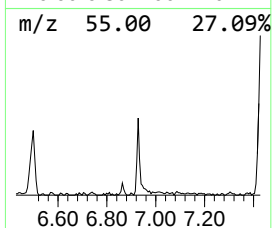
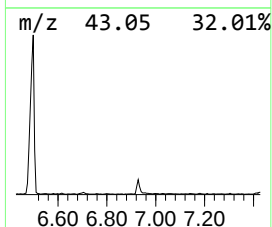
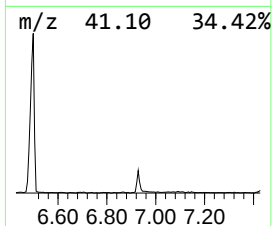
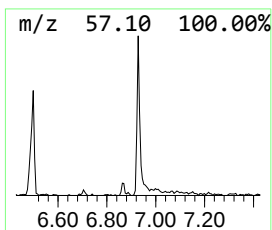
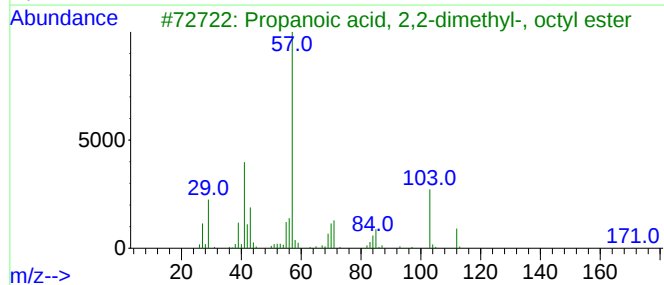
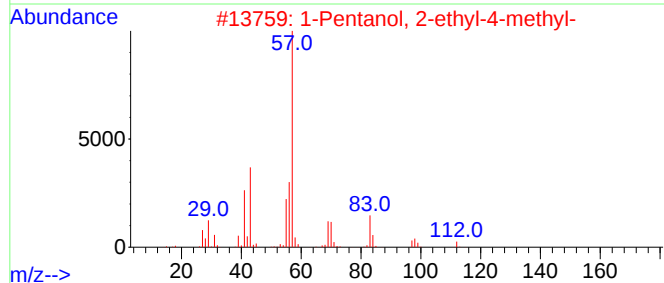
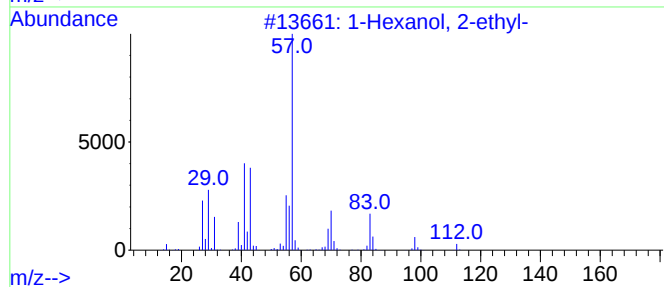
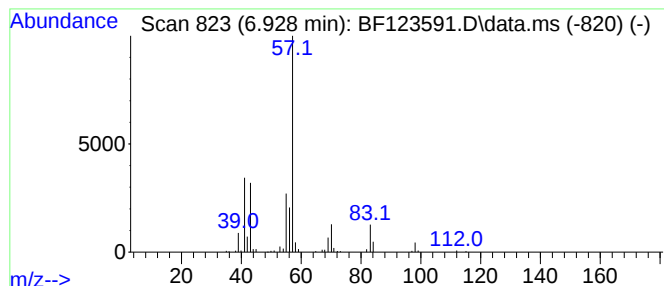
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	3.26 ng	208156	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	64
4			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
5			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50



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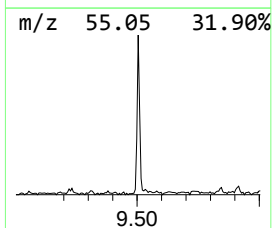
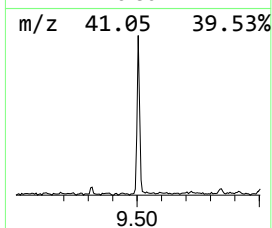
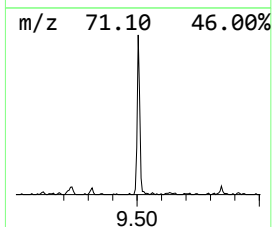
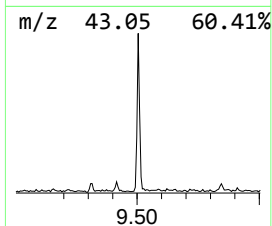
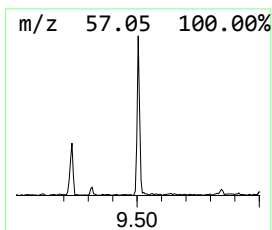
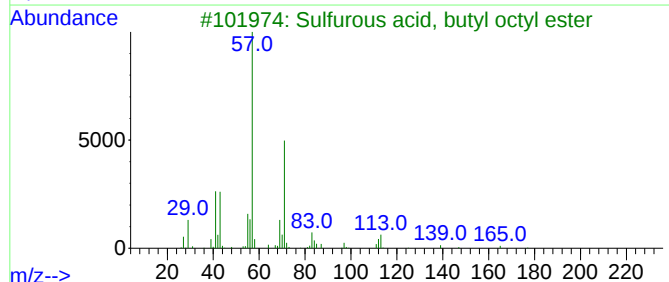
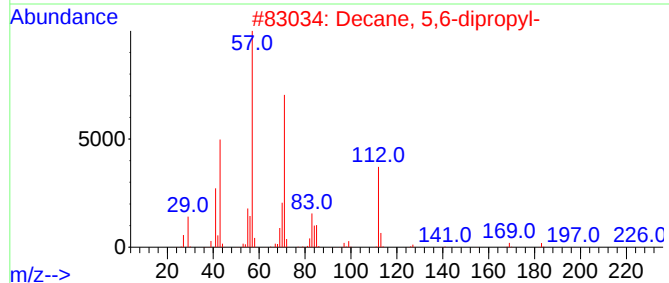
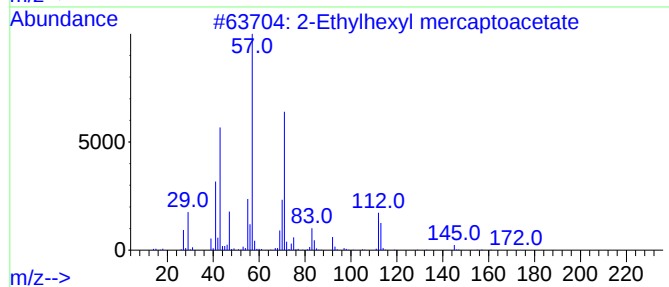
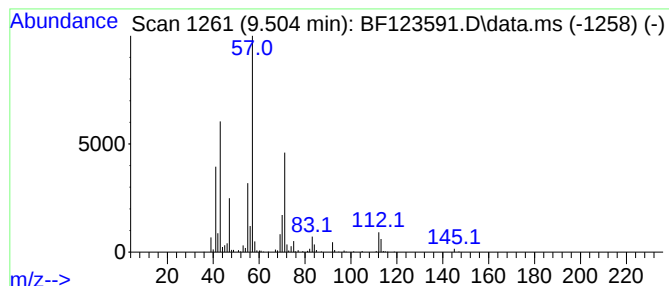
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Peak Number 4 2-Ethylhexyl mercaptoacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.504	5.35 ng	488569	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	83
2			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	53
3			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	53
4			Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	47
5			Octane, 3-ethyl-	142	C10H22	005881-17-4	47



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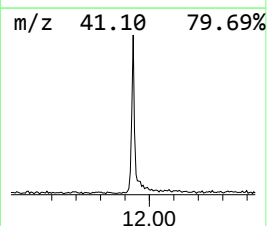
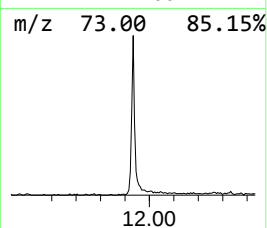
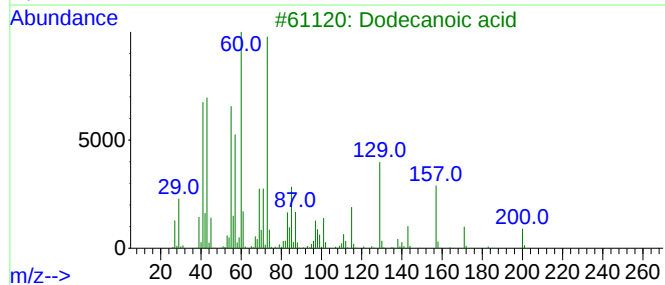
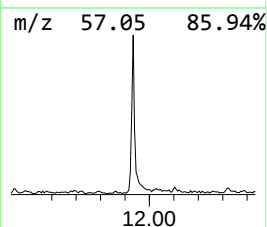
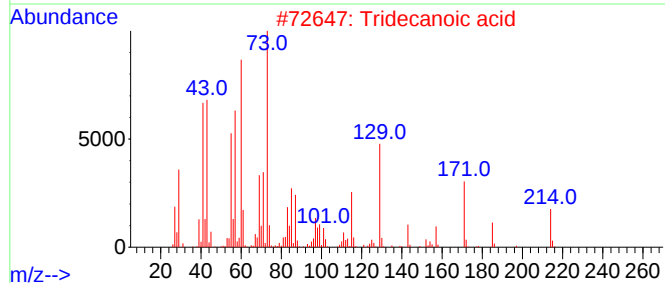
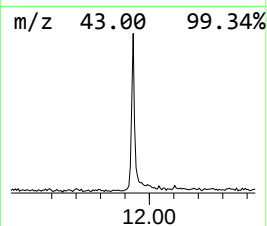
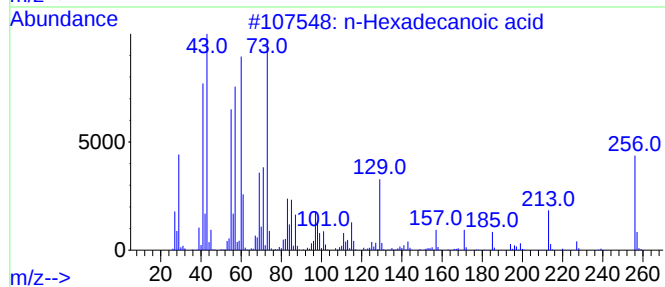
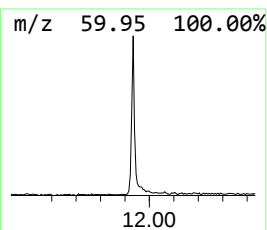
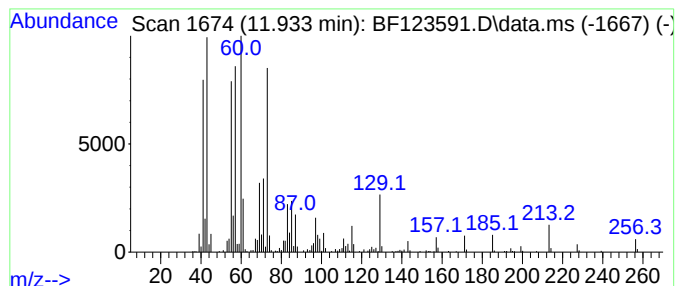
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	9.11 ng	915014	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Dodecanoic acid	200	C12H24O2	000143-07-7	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5			Oxalic acid, propyl tridecyl ester	314	C18H34O4	1000309-26-6	11



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Misc :
ALS Vial : 11 Sample Multiplier: 1

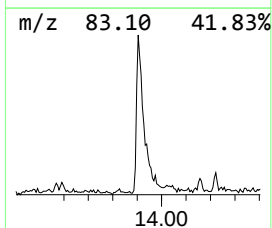
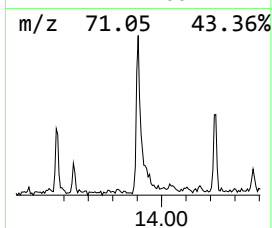
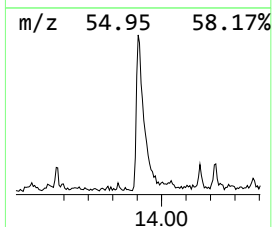
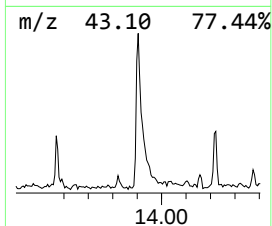
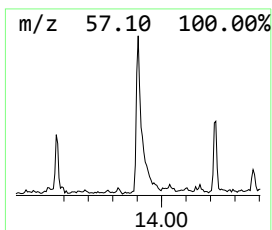
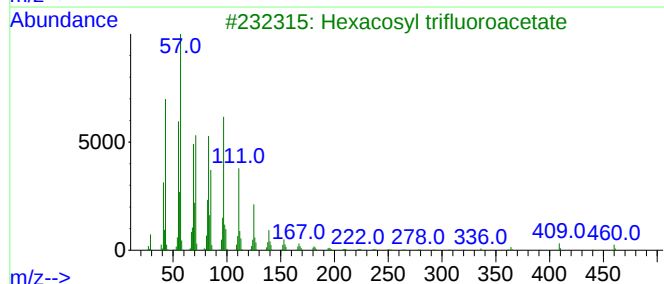
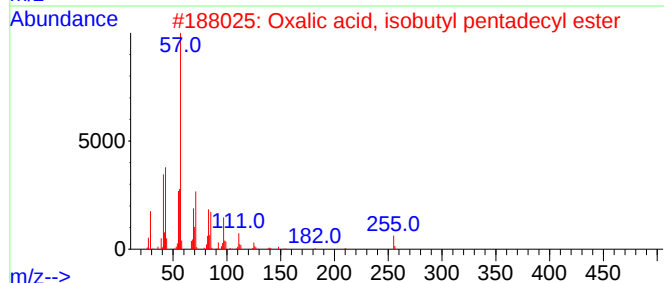
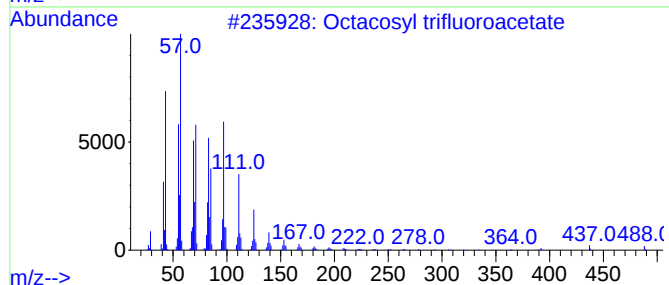
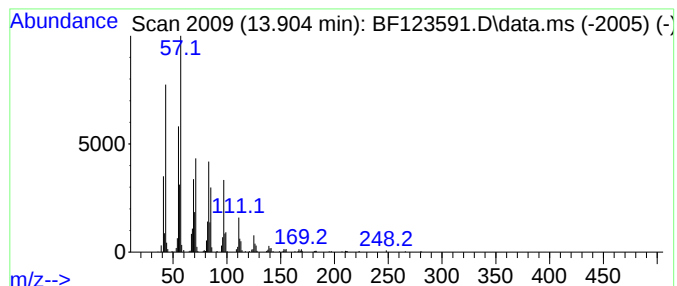
Instrument :
BNA_F
ClientSampleId :
SB-05-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.904	13.98 ng	1092070	Chrysene-d12		14.051	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate		506	C30H57F3O2	1000351-74-9	91
2	Oxalic acid, isobutyl pentadecyl...		356	C21H40O4	1000309-38-0	91
3	Hexacosyl trifluoroacetate		478	C28H53F3O2	1000351-75-0	90
4	Tetratriacontyl trifluoroacetate		591	C36H69F3O2	1000351-75-3	90
5	Triacetyl trifluoroacetate		534	C32H61F3O2	1000351-75-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123591.D
Acq On : 16 Apr 2021 14:20
Operator : JU/CG
Sample : M2048-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-05-14.5-15.0

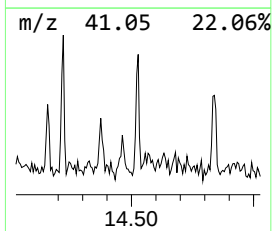
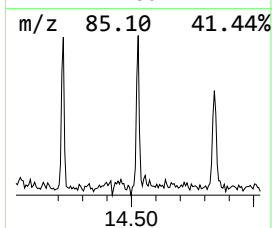
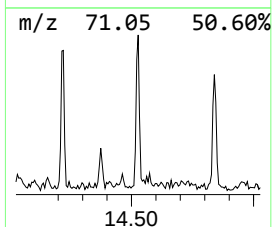
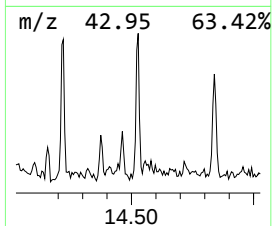
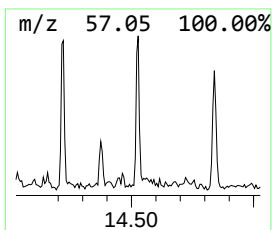
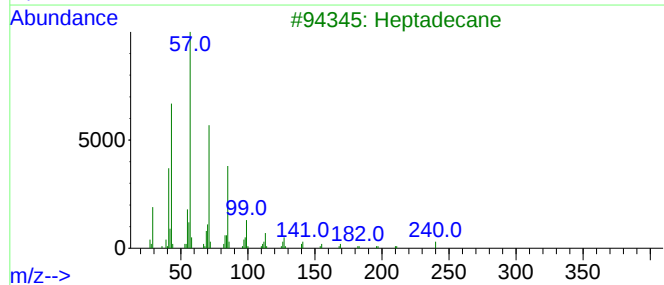
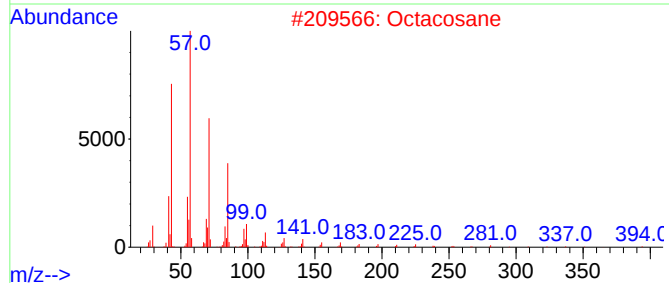
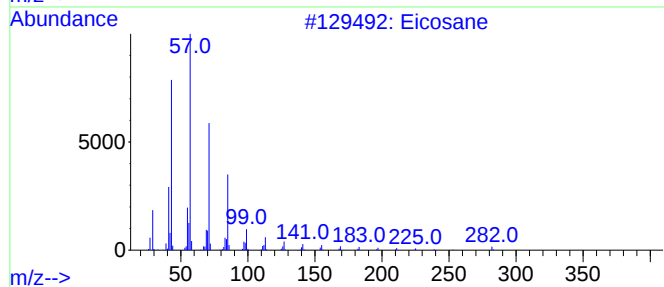
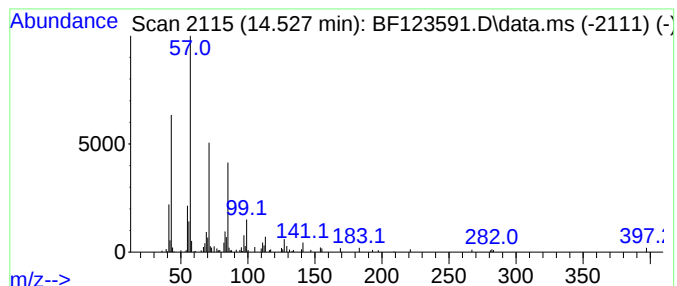
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	2.12 ng	165731	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Octacosane	394	C28H58	000630-02-4	87
3			Heptadecane	240	C17H36	000629-78-7	86
4			Tetracosane	338	C24H50	000646-31-1	86
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123591.D
Acq On : 16 Apr 2021 14:20
Operator : JU/CG
Sample : M2048-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-14.5-15.0

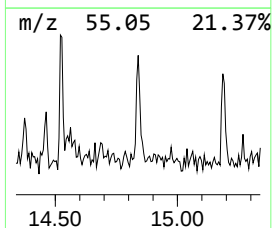
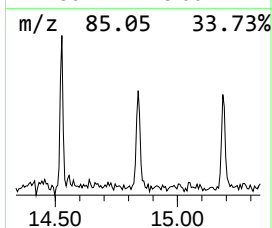
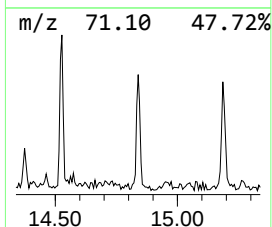
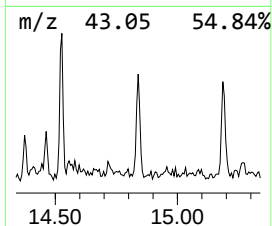
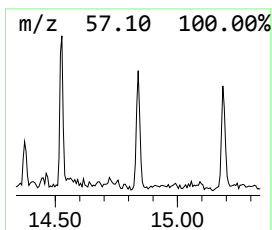
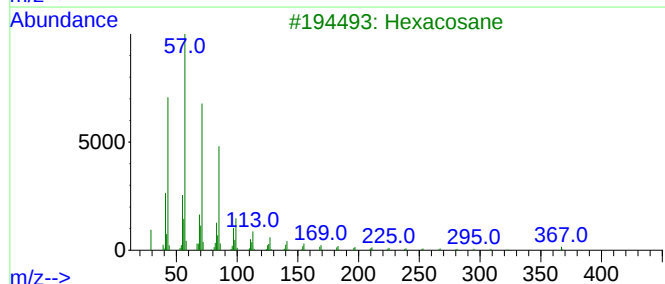
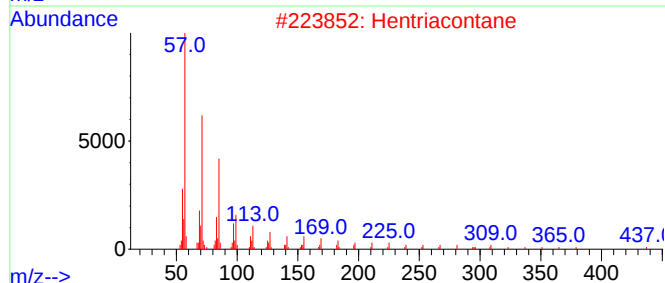
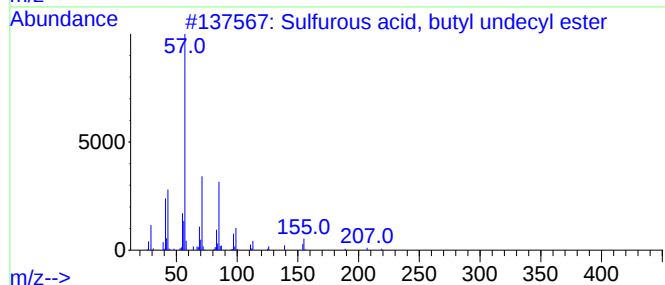
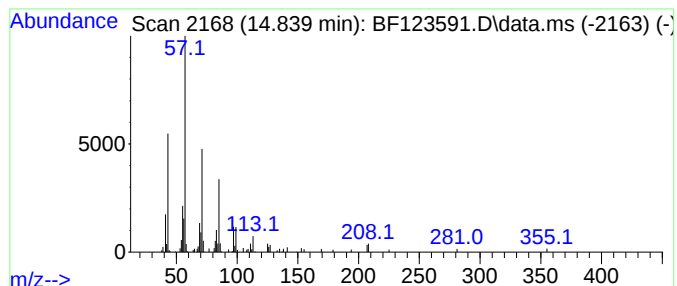
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Sulfurous acid, butyl undec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	2.70 ng	163967	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	80
2			Hentriacontane	437	C31H64	000630-04-6	72
3			Hexacosane	366	C26H54	000630-01-3	68
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5			Triacontane	422	C30H62	000638-68-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123591.D
Acq On : 16 Apr 2021 14:20
Operator : JU/CG
Sample : M2048-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-05-14.5-15.0

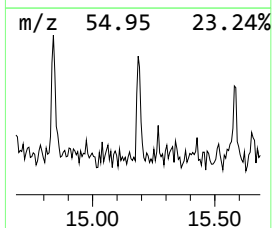
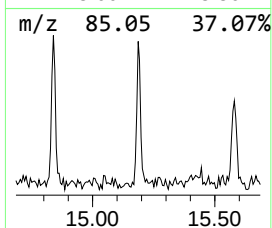
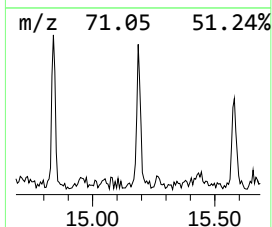
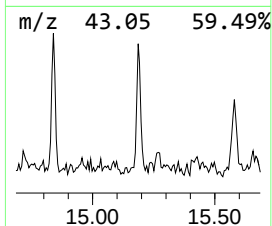
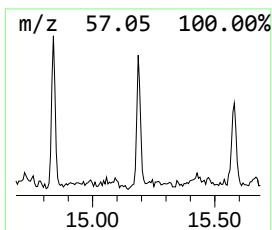
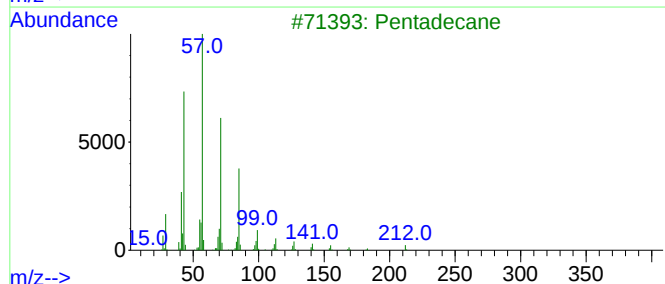
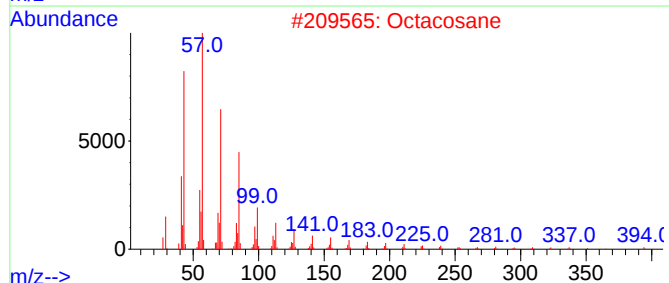
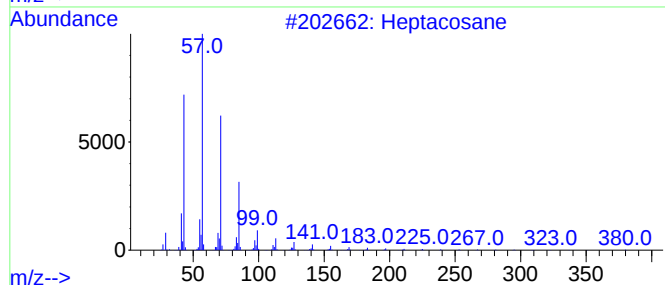
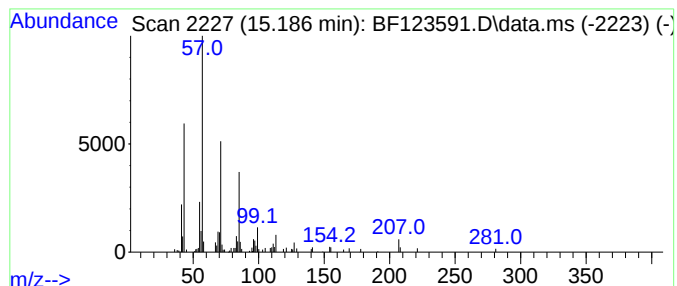
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	2.10 ng	127774	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Octacosane	394	C28H58	000630-02-4	86
3			Pentadecane	212	C15H32	000629-62-9	83
4			Heptadecane	240	C17H36	000629-78-7	80
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123591.D
Acq On : 16 Apr 2021 14:20
Operator : JU/CG
Sample : M2048-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.140	60.3	ng	3851720	1	6.869	1277500	20.0
2-Pentanone, 4-...	5.087	9.4	ng	598487	1	6.869	1277500	20.0
1-Hexanol, 2-et...	6.928	3.3	ng	208156	1	6.869	1277500	20.0
2-Ethylhexyl me...	9.504	5.3	ng	488569	3	9.910	1825260	20.0
n-Hexadecanoic ...	11.933	9.1	ng	915014	4	11.398	2008350	20.0
Octacosyl trifl...	13.904	14.0	ng	1092070	5	14.051	1562190	20.0
Eicosane	14.527	2.1	ng	165731	5	14.051	1562190	20.0
Sulfurous acid,...	14.839	2.7	ng	163967	6	15.539	1216340	20.0
Heptacosane	15.186	2.1	ng	127774	6	15.539	1216340	20.0